

MASS-ANALYZED THRESHOLD IONIZATION SPECTROSCOPY OF CYCLIC $\text{La}(\text{C}_5\text{H}_6)$ FORMED BY La ATOM ACTIVATION OF PENTYNE AND PENTADIENE

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La atom reactions with 1-pentyne ($\text{CH}\equiv\text{CCH}_2\text{CH}_2\text{CH}_3$) and 1,4-pentadiene ($\text{CH}_2=\text{CHCH}_2\text{CH}=\text{CH}_2$) were carried out in a laser-ablation molecular beam source. $\text{La}(\text{C}_5\text{H}_6)$ was observed in the two reactions through time-of-flight mass spectrometry and characterized by mass-analyzed threshold ionization spectroscopy. The most stable isomer of $\text{La}(\text{C}_5\text{H}_6)$ was identified as a six-membered metallacycle, $\text{La}(\text{CH}_2\text{CH}=\text{CHCH}=\text{CH})$, with La binding to the two terminal carbon atoms of the unsaturated hydrocarbon. The metallacycle is formed by hydrogen elimination and migration induced by the La atom. The neutral complex with C_1 symmetry has a doublet ground state, and the corresponding ion has a singlet state generated by the removal of a La 6s-based electron. The adiabatic ionization energy of the metallacycle was determined to be $37941(5) \text{ cm}^{-1}$. Three vibrational modes of the ion were measured to be 318, 407, and 538 cm^{-1} , which correspond to the La-ligand stretching, carbon skeleton bending with CH_2 rocking, and carbon skeleton bending with CH_2 twisting, respectively. In addition, two hot bands were observed at 276 and 367 cm^{-1} below the origin band and identified to be the vibrational frequencies of the La-ligand stretching and carbon skeleton bending with CH_2 rocking modes of the neutral complex.